Analysis of Multi-Scale Phenomena in Heterogeneous Materials

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Abstract

A new variational methodology is developed for computing optimal bounds on the stress inside thermoelastic composites. The method also provides tight bounds on the strength domains for random two-phase elastic-plastic composites. A second effort develops a global - local finite element method for problems with multiple length scales such as functionally graded thermal barrier coatings. The method consists of a global Galerkin scheme based upon the use of a small number of optimal local basis functions. The local bases are supported on sub domains of fixed diameter within the computational domain. A new class of optimal local bases are discovered that provide local approximations to the actual solution with exponentially decreasing error. For this choice the global Galerkin approximation converges exponentially with the coarse scale degrees of freedom. A third effort develops novel power series representations for TE and TM modes propagating through a two dimensional meta material crystal. The theory delivers an explicit relation between the geometry of the periodic scatters and the band structure of the crystal. This provides the opportunity to systematically design the location of double negative pass bands by tuning the geometry of the crystal.

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14. ABSTRACT

A new variational methodolo9gy is developed for computing optimal bounds on the stress inside thermoelastic composites. The method also provides tight bounds on the strength domains for random two phase elastic plastic composites. A second effort develops a global local infinite element method for problems with multiple length scales such as functionally graded thermal barrier coatings. The method consists of a global Galerkin scheme based upon the use of a small number of optimal local basis functions. The local bases are supported on sub domains of fixed diameter within the computational domain. A new class of optimal local bases are discovered that provide local approximations to the actual solution with exponentially decreasing error. For this choice the global Galerkin approimxation converges exponentially with the coarse scale degrees of freedom.

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Contents

1 Overview

In this research effort we seek to develop new mathematical and computational tools for the quantitative description of multi-scale phenomena seen in composite structures. The first research project develops a variational methodology for computing optimal bounds on the stress inside thermoelastic composites. The method also provides tight bounds on the strength domains for random two-phase elastic-plastic composites. This work is carried out together with the PI's former Ph.D. student Bacim Alali (University of Utah) and current Ph.D. student Yue Chen at LSU.

A second effort develops a numerical method for problems involving multiple length scales such as functionally graded thermal barrier coatings. Because of their multi-scale nature these problems have many degrees of freedom and one seeks numerical approaches based upon dimension reduction. Unfortunately in many cases no clear scale separation is present and "off the shelf" notions of homogenization do not apply. We address this problem and develop a multi-scale finite element method using a global Galerkin scheme based upon the use of a small number of optimal local basis functions. The local bases are supported on subdomains of fixed diameter within the computational domain and are determined by the local structure of the heterogeneous material. A new optimal class of local bases are discovered that provide local approximations to the actual solution with exponentially decreasing error. For this choice the global Galerkin approximation converges exponentially with the coarse scale degrees of freedom. This work is carried out in collaboration with Ivo Babuska at the University of Texas.

The third project focuses on the development of rigorous mathematical methods for the quantitative analysis of electromagnetic materials dubbed meta-materials. Novel power series representations for TE and TM modes propagating through a two dimensional meta material crystal made either from high dielectric rods or frequency dependent "plasmonic" rods are developed. The theory delivers convergent multi-scale expansions for each branch of the dispersion relation. The theory provides an explicit relationship between the geometry of the periodic scatters to the pass bands and stop bands of the crystal. This project has been carried out in collaboration with Stephen Shipman (LSU) and Santiago Fortes (LSU now at Caltech). We then show how to construct a metamaterial crystal with negative group velocity pass bands. To do this we identify a novel crystal constructed from high dielectric rods coated with a frequency dependent plasmonic coating. We develop a novel power series expansion for the TE modes inside the crystal. The power series representation is used as a tool to identify novel behavior. We show that the Mie resonances appearing in the first order term of the power series expansion interact with generalized electrostatic resonances appearing in the second order term to generate a dispersion relation with negative group velocity pass bands associated with double negative behavior. These results provide the opportunity for the systematic design of double negative pass bands by tuning the geometry of the crystal. This project has been carried out with Yue Chen who is a Ph.D. student at LSU and has been provided support under this grant.

Lastly we report on progress related to the characterization of field concentrations inside media with microstructure. Here the medium consists of multiple constituent materials each with distinct linearly elastic and heat conducting properties. New multi-scale methods developed by the PI under previous AFOSR support provide upper bounds on the L^∞ norms of gradients and fluxes inside heterogeneous media. The upper bounds are given by " modulation" functions relating gradients of homogenized fields to the L^∞ norms of the actual local gradient fields over a domain of interest. In this work we derive new lower bounds on the local L^∞ norms of local field gradients using the modulation functions and outline conditions under which the upper and lower bounds agree. The bounds are shown to naturally diverge when the microsturcture has cusps or reentrant corners. These results provide a methodology for extracting local field concentration information without having to solve the complete boundary value problem over the full domain. For periodic microstructures with smooth interfaces the upper and lower bounds are seen to agree and we obtain a representation formula for limits of sequences of L^∞ norms of thermal gradients associated with solutions of periodic microstructures in the fine phase limit. The formula for the limit is expressed in terms of the L^∞ norm of the local corrector problem inside the unit period cell. This corrector formula is the L^∞ norm analogy to the well known corrector formula for the effective energy see, for example [22]. To the best of the PI's knowledge this is the first formula of this type. This project is carried out with Tadele Mengesha at LSU.

The following Ph.D. students of the PI have been partially supported under this grant: Silvia Jimenez, Bacim Alali, Santiago Fortes, and Yue Chen. Presently Dr. Santiago Fortes is a research scientist at Caltech, Dr. Bacim Alali is a Wiley Assistant Professor at the University of Utah, Dr. Silvia Jimenez is a Visiting Assistant Professor at Worcester Polytechnic Insititute and Yue Chen is a Ph.D. student at LSU.

2 Summary of Research Projects

1 Optimal bounds on local field properties inside random composites

The majority of work on random heterogeneous media has focused on the characterization of the effective overall properties of the media. Such properties include the effective elastic, electric, magnetic and thermal properties of a heterogeneous medium. On the other hand it is very important to complement the theory of effective properties with new techniques for teasing out the relationships that connect the local field behavior inside a random medium to the macroscopic loads that are applied to it. These relationships provide a way to assess the likelihood of failure due to the presence of extreme local fields generated by an applied macroscopic load.

1 Optimal bounds on the stress inside thermoelastic composites

In this project the PI together with his Ph.D. student Yue Chen have developed new optimal lower bounds on the maximum local stress inside random heterogeneous thermoelastic media undergoing macroscopic thermomechanical loading. The methodology is based on a combination of convex analysis, cross-property relations and Hashin Shtrikman variational principles.

Here we consider mixtures of two thermoelastic materials with shear and bulk moduli specified by μ_1, k_1, μ_2, k_2 and coefficients of thermal expansion given by h_1 and h_2. The new lower bounds are shown to hold for elastically well ordered phases for which $k_1 > k_2$ and $\mu_1 > \mu_2$ as well as for non well ordered phases such that $k_2 > k_1$ and $\mu_1 > \mu_2$. To fix ideas we suppose $h_1 > h_2$ and $h_2 > h_1$ and we present lower bounds on the maximum value of the magnitude of the local hydrostatic stress $\sigma^{HS}(\mathbf{x})$ for points $\mathbf{x}$ inside a two phase composite occupying the unit cube Q. A constant macroscopic hydrostatic stress σ_0 and uniform change in temperature ΔT is imposed upon the heterogeneous material inside the cube. For each realization of the two-phase composite the local stress and strain are obtained from the solution of the standard thermoelastic boundary value problem [4]. Here we consider any two-phase thermoelastic medium with volume fractions of each material specified by θ_1 and θ_2. For this case we present optimal lower bounds on $\max_{\mathbf{x} \text{in} Q}\left\{|\sigma^{HS}(\mathbf{x})|\right\}$. The lower bounds are expressed in terms of the following parameter groups given by:

$$L_1 = \frac{k_1(k_2 + \frac{4}{3}\mu_2)}{k_1k_2 + (k_1\theta_1 + k_2\theta_2)\frac{4}{3}\mu_2}, \tag{1}$$

$$M_2 = \frac{k_2(k_1 + \frac{4}{3}\mu_2)}{k_1k_2 + (k_1\theta_1 + k_2\theta_2)\frac{4}{3}\mu_2}, \tag{2}$$

$$D = \Delta T(\frac{3k_1k_2(h_2 - h_1)}{k_2 - k_1}) \quad , \quad F = D(1 - \frac{1}{\frac{L_1+M_2}{2}}). \tag{3}$$

To fix ideas we suppose the two materials are elastically well ordered and consider the case $h_2 > h_1$ and the lower bounds are given in the following table.

Range	*LowerBound*
$-\infty < \sigma_0 \leq D$	$\max_{\mathbf{x}\text{in Q}}\left\{|\sigma^{HS}(\mathbf{x})|\right\} \geq \sqrt{3}[(D - \sigma_0)L_1 - D]$
$D \leq \sigma_0 \leq F$	$\max_{\mathbf{x}\text{in Q}}\left\{|\sigma^{HS}(\mathbf{x})|\right\} \geq \sqrt{3}[(D - \sigma_0)M_2 - D]$
$F \leq \sigma_0 < \infty$	$\max_{\mathbf{x}\text{in Q}}\left\{|\sigma^{HS}(\mathbf{x})|\right\} \geq \sqrt{3}[(\sigma_0 - D)L_1 + D]$

All of the lower bounds listed above are attained by the hydrostatic stress field inside a suitable coated sphere assemblage. In all there are 42 distinct lower bounds each associated with the relative magnitudes of the parameter groups D, F, L_1, M_2 as listed (together with their counterparts L_2 and M_1 obtained from L_1 and M_1 under a suitable change of index). Here the parameters D and F represent the effects of thermal expansion, while L_1, L_2, M_1, M_2 represent the purely elastic effects. In certain parameter regimes it is found that there are combinations of applied stress and imposed temperature change for which the local hydrostatic stress inside the connected phase of the coated sphere assemblage vanishes identically. Other loading combinations are seen to cause the stress inside the included phase of the coated sphere assemblage to vanish identically. Thus for these cases the applied hydrostatic stress is converted into a pure local shear stress inside a preselected phase. The methodology together with the full set of bounds have appeared in Acta Mechanica 213, 97109 (2010) DOI 10.1007/s00707-009-0273-1.

2 Tight bounds on the strength domains for random two-phase elastic-plastic composites

In many instances one does not have access to the underlying probability measure describing the random elasticity tensor field and instead one must make use of partial statistical information describing the random microstructure. In this paper we address the case when only the volume fractions of the two materials are known. For a given realization of the random medium, the theory of failure initiation posits that failure is initiated when certain rotational invariants of the local elastic stress exceed threshold values [2]. An example is an elastic–perfectly plastic material. Here the material deforms elastically up to some threshold value and then yields undergoing plastic, or irreversible deformation [3]. Typical stress invariants used to describe failure include the local hydrostatic stress component σ^H which measures the hydrostatic force acting inside the material and the Von Mises equivalent stress σ^V which measures the local shearing forces acting inside a material [2].

The shear and bulk moduli of materials one and two are denoted by μ_1, μ_2 and κ_1, κ_2 respectively. To fix ideas we suppose that the two materials are elastically well ordered, i.e., $\mu_1 > \mu_2$ and $\kappa_1 > \kappa_2$. The volume fractions of materials one and two are specified by θ_1 and θ_2. For the first example the composite is subjected to an applied uniform pure shear stress of the form $\overline{\sigma}^D_{ij} = s(\mathbf{a_i b_j} + \mathbf{a_j b_i})$, where s is the magnitude of the applied stress and the shear components are specified the unit vectors $\mathbf{a}$ and $\mathbf{b}$ which are are orthogonal. In this example no volume fraction constraints are imposed and we consider the macroscopic strength domain K^{Safe} defined to be the set of all applied stresses $\overline{\sigma}^D$ for which the local Von Mises stress satisfies the local stress constraints given by $\sigma^V(\mathbf{x}) < F_1$ inside material one and $\sigma^V(\mathbf{x}) < F_2$, in material two. Now we define $\overline{K}$ to be the set of matrices of the form $\overline{\sigma}^D = s(\mathbf{a} \odot \mathbf{b})$ that satisfy the constraint given by $|\overline{\sigma}^D| \leq \min(F_1, F_2)$ and we have the following tight upper bound.

Upper bound on the macroscopic strength domain for deviatoric applied loads

Suppose $F_1 \leq F_2$ then $K^{Safe} \subset \overline{K}$. Moreover $\overline{K}$ is a tight upper bound in that $\overline{\sigma}^D \in \overline{K}$ implies that the local deviatoric component of stress $\sigma^V(\mathbf{x})$ lies below the failure threshold inside both phases for a simple layered material with layer normal chosen parallel to $\mathbf{a}$ or $\mathbf{b}$. And $\overline{\sigma}^D \notin \overline{K}$ implies that the threshold has been exceeded everywhere inside phase one of the layered material.

Next we display an upper bound on the strength domain associated with norm of the full local stress $\sigma(\mathbf{x})$ inside the composite. This norm is the given by the square root of sum of the squares of all components of the stress tensor and is denoted by $|\sigma(\mathbf{x})|$. We suppose that failure is initiated inside phase one when $|\sigma(\mathbf{x})| = F_1$ over some subset of phase one and inside phase two when $|\sigma(\mathbf{x})| = F_2$ over some subset of phase two. We suppose that only the volume fractions θ_1 and θ_2 are known. For this case we impose a macroscopic hydrostatic stress $\overline{p}$ and we define the macroscopic strength domain K^{Safe} to be the set of applied stresses $\overline{p}$ for which the stress field inside the composite $\sigma(\mathbf{x})$ satisfies the local constraints $|\sigma^V(\mathbf{x})| < F_1$ in material one and $|\sigma^V(\mathbf{x})| < F_2$ in material two. We write

$$L_1(\theta_1) = \frac{\sqrt{3}(\kappa_1\kappa_2 + \frac{4}{3}\mu_2\kappa_1)}{\kappa_1\kappa_2 + \frac{4}{3}\mu_2(\theta_1\kappa_1 + \theta_2\kappa_2)} \text{ and}$$

$$L_2(\theta_1) = \frac{\sqrt{3}(\kappa_1\kappa_2 + \frac{4}{3}\mu_1\kappa_2)}{\kappa_1\kappa_2 + \frac{4}{3}\mu_1(\theta_1\kappa_1 + \theta_2\kappa_2)} \tag{4}$$

(5)

and define the upper bound $\overline{K}$ to be the set of matrices of the form $\overline{p}I$ that satisfy the constraints given by $|\overline{p}|L_1(\theta_1) \leq F_1$ and $|\overline{p}|L_2(\theta_1) \leq F_2$.

We now present a tight upper bound on K^{Safe}.

Upper bound on the macroscopic strength domain for hydrostatic applied loads

Suppose that $F_1 \leq F_2$ then $K^{Safe} \subset \overline{K}$. Moreover $\overline{K}$ is a tight upper bound in that $\overline{p} \in \overline{K}$ implies that the local stress $|\sigma(\mathbf{x})|$ lies below the failure threshold inside both phases for the coated sphere construction with core material one and coating material two. And $\overline{p} \notin \overline{K}$ implies that the threshold has been exceeded everywhere inside the core phase of the coated sphere assemblage. These results are obtained in joint work with Bacim Alali and have appeared in SIAM Journal on Applied Mathematics, 70, 2009, pp. 1260–1282.

2 Generalized finite element methods for multiscale problems

Large multi-scale systems such as airplane wings and wind turbine blades are built from fiber reinforced composites and exhibit a cascade of substructure spread across several length scales. These and other large composite structures are now seeing extensive use in transportation, energy, and infrastructure. The importance of accurate numerical simulation is ever increasing due to the high cost of experimental testing of large structures made from heterogeneous materials. The computational modeling of such heterogeneous structures is a very large problem that requires the use of parallel computers. In order for a numerical method to be adequate it must be able to utilize many local computations performed independently on single processors or clusters of processors of reasonable size. Additionally because of their multi-scale nature these problems have many degrees of freedom and one seeks numerical approaches based upon dimension reduction. Unfortunately in many cases no clear scale separation is present and "off the shelf" notions of homogenization do not apply. We address both the problems of parallelization and dimension reduction and develop a multi-scale finite element method using a global Galerkin scheme based upon the use of a small number of optimal local basis functions. The local bases are supported on subdomains of fixed diameter within the computational domain and are determined by the local structure of the heterogeneous material. The notion of the Kolmogorov n-width is used to characterize new optimal class of local bases. It is shown that these bases provide local approximations to the actual solution with exponentially decreasing error. For this choice the global Galerkin approximation converges exponentially with the coarse scale degrees of freedom. When length scales "separate" and the microstructure is sufficiently fine with respect to the length scale of the local domain it is shown that homogenization theory can be used to construct local approximation spaces with exponentially decreasing error in the pre-asymtotic regime.

Future work will apply and further refine these methods to model functionally graded thermal barrier coatings in the presence of prestresss. This is joint work with Ivo Babuska at the University of Texas. These results will appear in SIAM Multiscale Modeling and Simulation 2011.

3 Power series representations for TE and TM modes propagating through two dimensional meta material crystals.

1 TE mode propagation inside sub-wavelength plasmonic crystals

Sub-wavelength plasmonic crystals are a class of *meta-material* that possesses a microstructure consisting of a periodic array of plasmonic inclusions embedded within a dielectric host. The term "sub-wavelength" refers to the regime in which the period of the crystal is smaller than the wavelength of the electromagnetic radiation traveling inside the crystal. Many recent investigations into the behavior of meta-materials focus on phenomena associated with the *quasi-static limit* in which the ratio of the period cell size to wavelength tends to zero. Sub-wavelength micro-structured composites are known to exhibit effective electromagnetic properties that are not available in naturally-occurring materials. Here we obtain a convergent power series expansion for the first branch of the dispersion relation for subwavelength plasmonic crystals consisting of plasmonic rods with frequency-dependent dielectric permittivity embedded in a host medium with unit permittivity. The expansion parameter is $\eta = kd = 2\pi d/\lambda$, where k is the norm of a fixed wavevector, d is the period of the crystal and λ is the wavelength, and the plasma frequency scales inversely to d, making the dielectric permittivity in the rods large and negative. The expressions for the series coefficients (a.k.a., dynamic correctors) and the radius of convergence in η are explicitly related to the solutions of higher-order cell problems and the geometry of the rods. Within the radius of convergence, we are able to compute the dispersion relation and the fields and define dynamic effective properties in a mathematically rigorous manner. Explicit error estimates show that a good approximation to the true dispersion relation is obtained using only a few terms of the expansion. The convergence proof requires the use of properties of the Catalan numbers to show that the series coefficients are exponentially bounded in the H^1 Sobolev norm. This is joint work with Stephen Shipman (LSU) and Santiago Fortes (LSU). This work has appeared in The Proceedings of the Royal Society of London, Published on line Feb. 10, 2010 doi: 10.1098/rspa.2009.0542.

2 High dielectric sub-wavelength metamaterials

We obtain convergent power series representations for Bloch waves in periodic high-contrast media. The material coefficient in the inclusions can be positive or negative. The small expansion parameter is the ratio of period cell width to wavelength, and the coefficient functions are solutions of the cell problems arising from formal asymptotic expansion. In the case of positive high dielectric coefficients, the dispersion relation has an infinite sequence of branches, each represented by a convergent even power series whose leading term is a branch of the dispersion relation for the homogenized medium. This is joint work with Santiago Fortes (LSU) and Stephen Shipman (LSU). This work has appeared in Communications in Partial Differential Equations 36, 2011, pp. 1016–1043.

3 Construction of sub-wavelength metamaterials with negative group velocity pass bands

Metamaterials are new class of man made materials that impart unconventional electromagnetic properties derived from sub-wavelength configurations of different conventional materials [5]. The first such materials were seen to exhibit behavior associated with negative bulk dielectric constant [6] and were constructed from a cubic lattice of metal wires. Subsequently negative effective magnetic permeability at microwave frequencies were derived from periodic arrays of non-magnetic metallic split ring resonators [5]. Double negative or left handed metamaterials with simultaneous negative bulk permeability and permittivity at microwave frequencies have been developed using periodic arrays of metallic posts and split ring resonators [7]. Subsequent work has delivered several new designs using different configurations of metallic resonators for double negative behavior [8, 9, 10, 11, 12, 13, 14, 15, 16].

For higher frequencies in the infrared and optical range an alternate strategy for constructing negative effective permeability from non-magnetic components relies on Mie resonances associated with small rods or particles made from high permittivity materials [17, 18].

A double negative metamaterial may be achieved by coating the high permittivity material with a metallic coating having frequency dependent dielectric constant with plasmonic or Drude type behavior at optical frequencies [19, 20, 21].

In this project we focus on the second approach and propose periodic assemblages of aligned non-magnetic dielectric rods each clad with a non-magnetic plasmonic coating. For this case we are able to explicitly calculate the propagation band structure in the sub-wavelength limit. The pass bands and stop bands are given by formulas that depend explicitly on the rod diameters and coating thickness. We show how to construct tunable pass bands associated with double negative effective properties. The physical origin of the negative effective permeability is due to the excitations of Mie resonances inside the rods. On the other hand the negative effective permittivity is caused by the electrostatic resonance excited near the plasma resonance of the coating. We provide the explicit relationship linking Mie resonances and the frequency dependent effective permittivity to the spacing of the rods, the rod radii, and the coating thickness for the coated rod assemblage proposed here.

These relationships are found not by appealing to effective medium theory based on the Clausius-Mossotti formula, but instead we show that it is profitable to take a different approach and characterize wave propagation using explicit multiscale expansions for waves inside the metamaterial crystal. The wave number associated with a Bloch wave inside the d-periodic crystal is denoted by $k = 2\pi/\lambda$ where λ is the wavelength. The approach taken here provides an explicit power series expansion for the fields in the parameter $\eta = dk$. We outline a systematic framework in which the homogenized dispersion relation is recovered directly from the expansion in the subwavelength $d << \lambda$ limit. We introduce metamaterial crystals made from coated rod assemblages and obtain explicit homogenized dispersion relations for these geometries. The dispersion relations provide explicit conditions on the the distance between neighboring rods, rod radii, and coating thickness necessary for generating pass bands associated with double negative behavior. Two examples are provided showing how the band structure can be manipulated to generate double negative pass bands with negative group velocity. This is joint work with Yue Chen (LSU). This work has appeared in New Journal of Physics 12 (2010) 083010.

4 Representation formulas for L^∞ norms of weakly convergent sequences of gradient fields in homogenization

Together with Tadele Mengesha (LSU) we examine the composition of the L^∞ norm with sequences of gradient fields associated with the homogenization of second order divergence form partial differential equations. Here the sequences of coefficients are chosen to model heterogeneous media and are piecewise constant and highly oscillatory. We identify a set of local representation formulas that in the fine phase limit that provide lower bounds on the limit superior of the L^∞ norms of gradient fields. The representation formulas are given by " modulation" functions relating gradients of homogenized fields to the L^∞ norms of the local gradient inside a preselected domain. Earlier AFOSR supported work by the PI developed upper bounds for the limit superior of the sequence of L^∞ norms. The upper and lower bounds naturally diverge when the microstructure has cusps or reentrant corners. For periodic microstructures with smooth interfaces we derive a representation formula for limits of sequences of L^∞ norms of thermal gradients associated with solutions of periodic microstructures in the fine phase limit. The formula for the limit is expressed in terms of the L^∞ norm of the local corrector problem inside the unit period cell.

Because of its novelty we will give the necessary background and present the formula. The unit period for the microstructure Y contains a collection of smooth particles with $C^{1,\alpha}$ boundaries separated by matrix material. The coefficient $A(\mathbf{y})$ is a periodic function defined on the unit period cell Y taking the value α inside each particle and β in the matrix. Rescaling gives the sequence of coefficients $A(\mathbf{x}/n)$, $n = 1, 2, \ldots$, corresponding to progressively finer periodic microstructures. The temperature fields u^n associated with the sequence of coefficients solve the boundary value problems inside the domain of interest D given by

$$-\text{div}\,(A(\mathbf{x}/n)\nabla u^n) = 0 \tag{6}$$

with $u^n = U$ on the boundary of D. The theory of periodic homogenization [22], states that the averages of the sequence of solutions u^n and their gradients ∇u^n converge to the averages of the homogenized solution u^H and gradient ∇u^H that solves the *homogenized* boundary value problem $u^H = U$ on the boundary of D and

$$-\text{div}\left(A^H \nabla u^H\right) = 0, \text{ inside } D. \tag{7}$$

Here the constant matrix A^H of effective properties is given by the well known formula

$$A^H_{ij} = \int_Y A_{ik}(y) P_{kj}(y) dy \tag{8}$$

where $P_{kj} = \partial_{x_k}\phi^j(y) + \delta_{kj}$ and ϕ^j are Y-periodic solutions of the unit cell problems

$$\text{div}(A(y)(\nabla\phi^j(y) + \mathbf{e}^j)) = 0, \text{ in } Y, \tag{9}$$

and $\mathbf{e}^j$ $j = 1, 2, 3$ are orthonormal unit vectors. It is well known that the associated average energies taken over $S \subset D$ converge, i.e.,

$$\begin{aligned}\lim_{n\to\infty}\int_S A^n \nabla u^n \cdot \nabla u^n dx &= \int_S A^H \nabla u^H \cdot \nabla u^H dx \\ &= \int_{S\times Y} A(y)P(y)\nabla u^H(x)\cdot\nabla u^H(x)\, dydx. \end{aligned} \tag{10}$$

In this supported research we show *(for the first time)* that the analogous formulas hold for L^∞ norms and are given by the local representation formulas

$$\lim_{n\to\infty}\|\nabla u_n\|_{L^\infty(S)} = \|P(y)\nabla u^H(x)\|_{L^\infty(S\times Y)}. \tag{11}$$

We point out that previous related results have been developed by the PI over the course of several years of AFOSR support and provide the mathematical underpinnings (and generalization) for the *micro-mechanical enhancement to the strain invariant failure theory* developed at Boeing Aircraft Company by Gosse and Christensen, [23]. The present work has been submitted for publication in Mathematical Modeling and Numerical Analysis.

3 Publications resulting from the supported research

1. Babuska, I. and Lipton, R. "L^2 global to local projection: an approach to multiscale analysis," To appear in M3AS (2011).

2. Lipton, R. and Mengesha, T. " Representation formulas for L-infinity norms of weakly convergent sequencies of gradient fields in homogenization." arXiv:1009.4429v2 [math.AP] 23 Sep 2010.

3. Fortes, S., Lipton, R. and Shipman, S., "Convergent Power Series for Fields in Positive or Negative High-Contrast Periodic Media," Communications in Partial Differential Equations 36, 2011, pp. 1016–1043.

4. Chen, Y, and Lipton, R. "Tunable double negative band structure from non-magnetic coated rods," New Journal of Physics 12 (2010) 083010.

5. Alali, B. and Lipton, R. "Multiscale analysis of heterogeneous media in the peridynamic formulation," Journal of Elasticity (Online first), Dec. 8, 2010, pp. 1–33. DOI 10.1007/s 10659-010-9291-4.

6. Babuska, I. and Lipton, R. "Optimal local approximation spaces for generalized finite element methods with application to multiscale problems," to appear in Multiscale Modeling and Simulation, SIAM.

7. Jimenez, S. and Lipton, R. "Correctors and field fluctuations for the $p_\epsilon(x)$-Laplacian with rough exponents," J. Math. Anal. Appl. 372 2010, pp. 448–469.

8. Chen, Y. and Lipton, R. "Optimal lower bounds on the local stress inside random thermoelastic composites," Acta Mechanica. DOI 10.1007/s00707-009-0273-1, 15 Jan. 2010.

9. Fortes, S., Lipton, R., and Shipman, S. "Sub-wavelength plasmonic crystals: dispersion relations and effective properties," Proc. Roy. Soc. London A. Published on line Feb. 10, 2010 doi: 10.1098/rspa.2009.0542.

10. Alali, B. and Lipton, R. "Optimal lower bounds on local stress inside random media," SIAM Journal On Applied Mathematics 70, 2009, pp. 1260–1282.

11. Lipton, R. and Stuebner M. "A new method for design of composite structures for strength and stiffness." American Institute of Aeronautics and Astronautics Paper AIAA 2008-5986.

12. Babuska, I., Lipton, R. and Stuebner, M. "The penetration function and its application to microscale problems." *BIT Numerical Mathematics.* **48**, 2008, pp. 167–187.

4 Interactions/Transitions

1 Interactions with Government Laboratories

Since May of 2000 the PI has been interacting with the research team in the Laboratory at Wright Patterson Air Force Base lead by Dr. Tia Benson Tolle. As of Spring of 2001 the PI has also been collaborating with Dr. Greg Schoeppner (WPAFB) and Dr. Endel Iarve (UDRI contractor with WPAFB. One of the principle objectives of this interaction is the characterization of stress concentrations in composite materials. More recently the PI together with Dr. Tim Breitzman (WPAFB), Dr. Endle Iarve and Dr. Greg Schoeppner have embarked on the development of a fast multiscale numerical method for accurate stress assessment in prestressed composite materials used in aircraft. This methodology is being applied to the design of composite repair patches for high performance aircraft. The stress analysis method developed under this support, together with E. Iarve (UDRI) and T. Breitzman (AFRL, WPAFB), has been incorporated into a micromechanical failure criterion evaluation algorithm and transitioned to Sikorski Aircraft, Stratford, CT. Point of contact at Sikorski Aircraft is Jeffrey R. Schaff Structural Methods and Prognostics Group Sikorski Aircraft. 6900 Main Street, Stratford, CT, Phone: 203-386-7423.

2 Plenary Talks and Special Presentations

- "Failure Initiation and Uncertainty Inside Multi-Scale Random Media," (Keynote Lecture). 8^{th} World Congress on Computational Mechanics, June 30–July 4, 2008, Venice Italy.

- "Multi-Scale Stress Analysis Inside Heterogeneous Media and Macroscopic Failure Criteria," (Keynote Lecture). First American Academy of Mechanics Conference, New Orleans, Louisiana, June 17–20, 2008.

- "Optimal Design for Stress Control: Explicit Parametrization Via Inverse Homogenization," (Keynote Lecture). IV European Conference on Computational Mechanics, Paris France, May 16-21, 2010.

- "On Local-Global Approximation Error for GFEM," (Keynote Lecture). 9^{th} World Congress on Computational Mechanics, Sydney Australia, July 19-23, 2010.

- "Multiscale Structural Optimization in the Presence of Uncertainty for Very Large Composite Structures," Institute for Mathematics and Its Applications, Workshop: Computing with Uncertainty, October 18-22, 2010, Minneapolis, MN.

- "Multiscale Dynamics of Heterogeneous Media in the Peridynamic Formulation," Mini-workshop on Mathematical Analysis for Peridynamics, Mathematisches Forschungsinstitut Oberwolfach, January 16–22, 2011.

3 Graduate Student Support

- Ph.D. adviser for Bacim Alali, LSU, supported during the period 3/01/2008–8/15/2008. Dr. Alali received his Ph.D. August of 2008. He has a 3 year Wiley Instructor/Assistant Professor position at the Mathematics Department at the University of Utah.

- Ph.D. adviser for Santiago Fortes, LSU, supported during the period 1/25/2009-5/15/2010. Dr. Fortes is currently a Research Postdoctoral Assistant at the Department for Applied and Computational Mathematics at Caltech.

- Ph.D. adviser for Silvia Jimenez, LSU, supported during the period 8/15/2008-12/25/2008. Dr. Jimenez is now a visiting Assistant Professor at WPI from Fall 2010–Spring 2013.
- Ph.D. adviser for Yue Chen, LSU, supported during the period 5/15/2010-11/30/2010. Yue is currently a Ph.D. research assistant at LSU.

4 Presentations

Invited talks at academic institutions.

1. ICES Seminar, Institute for Computation and Engineering Sciences, University of Texas, Austin, TX, December 2010.
2. Mathematics Colloquium, Department of Mathematics University of Houston, Houston, TX, September 2010.
3. Mathematics Colloquium, Department of Mathematics University of Tennessee, Knoxville, TN, April, 2009.
4. Computational Science Seminar, Florida State University, Tallahassee, FL, April 2009.
5. Numerical Analysis Seminar, University of Maryland Department of Mathematics, College Park MD, December 2008.
6. Computational Modeling Seminar, Sandia National Laboratories, Albuquerque, NM, November 2008.
7. Mathematics Seminar, University of Rome I, Rome Italy, June 2008.
8. Department of Mechanical Science and Engineering Seminar, University of Illinois Urbana-Champaign, February 2008.

Invited talks at Conferences and Workshops.

1. "Dispersion Relations for Sub-wavelength Plasmonic Crystals & Meta Materials," Progress in Electromagnetics Research Symposium PIERS, July 2010, Cambridge, MA
2. "Optimal Lower Bounds on the Local Stress Inside Thermoelastic Composites," 16^{th} US National Congress on Theoretical and Computational Mechanics, State College, PA, June 2010.
3. "Macroscopic Strength Domains for Statistically Defined Heterogeneous Media," 16^{th} US National Congress on Theoretical and Computational Mechanics, State College, PA, June 2010.
4. "Tight Bounds on Failure Surfaces for Random Elastic-Plastic Composites," SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA May 2010.
5. "Sub-Wavelength Plasmonic Crystals: Dispersion Relations and Effective Properties," SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA May 2010.

6. "Dispersion Relations for Subwavelength Plasmonic Crystals," 2010 Spring AMS Southeastern Sectional Meeting Lexington, KY March 2010.

7. " Multiscale Modeling for Heterogeneous Peridynamic Media," IAMCS Workshop on Computational and Mathematical Challenges in Material Science and Engineering, Texas A&M University, December 2–3, 2009.

8. "Multi-scale Analysis of Peridynamics for Composite Media," US National Congress on Computational Mechanics USNCCM-10, Columbus Ohio July 2009.

9. "A New Method for Design of Composite Structures for Strength and Stiffness," US National Congress on Computational Mechanics USNCCM-10, Columbus Ohio July 2009.

10. "Controlling dispersion relations of frequency dependent materials near resonance," Symposium on Optimal Design in Electromagnetics, Society for Industrial and Applied Mathematics (SIAM) Annual Meeting, Denver, July 6-10, 2009.

11. "A New Method for Design of Composite Structures for Strength and Stiffness," World Congress on Structural and Multidisciplinary Optimization, WCSMO-8 Lisbon Portugal, June 1–5, 2009.

12. Meshless Methods, Generalized Finite Element Methods, and Related Approaches, University of Maryland, College Park, Maryland, March 26–27, 2008.

13. 12^{th} AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Victoria, BC, September 10–12, 2008.

14. Materials Science Program Review, Dayton Ohio, July 30-31, 2008.

15. 2008 SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia Pennsylvania, May 11–14.

16. 6^{th} International Conference on Mechanics of Time Dependent Materials, Monterey, CA, March 30–April 4, 2008.

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